MAR11-2010-005750

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Magnetic Moment and Electronic Correlations in Chemically Functionalized Graphene

JORGE SOFO, Penn State

Magnetic moments in extended systems are the result of local electronic correlations. In the case of graphene functionalized with chemisorbed atoms such as hydrogen, fluorine, or oxygen, the Anderson Model picture, where correlations in a localized state are responsible for the formation of a magnetic moment, has to be modified to properly describe the magnetic moment formation and their interactions. We use a tight-binding model with local correlations to analyze the results obtained with Density Functional Theory calculations for these systems. The model allows the treatment of local correlations beyond the mean field level and the investigations of a possible Kondo effect. We find that the Coulomb repulsion at the carbon atoms near the impurity play a crucial role in the magnetic moment formation. External doping with a gate voltage can control the nature of the binding and the formation of the magnetic moment. This effect could be observed in transport experiments as the scattering of the graphene electrons at the Fermi energy strongly depends on the structure of the defect.